PACE
PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Argonne NATIONAL LABORATORY
Sandia National Laboratories

Direct Numerical Simulation (DNS) and High-Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In-Cylinder Flow and Combustion Processes

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*Now at GE Global Research

2020 DOE Vehicle Technologies Office Annual Merit Review
June 1-4, 2020
Project # ACE146

Overview

Timeline

- **PACE started in Q3, FY19**
- **PACE will end in FY23 (~25% complete)**
- **Focus and objectives of individual tasks will be continuously adjusted**
- **Overall PACE work plan discussed in ACE138**

US Fiscal years run from October 1 through September 30

Budget

Results from three PACE projects

Task	FY19	FY20
F.02.01 High-fidelity engine simulations using Nek5000 code (ANL, Ameen)	$700k	$700k
E.02.01 DNS of flame propagation, wall quenching and soot formation (SNL, Chen)*		$100k
D.01.04 Simulation of soot formation from wall films (SNL, Nguyen)*		$100k

***Newly funded in FY20**

Barriers

<u>US DRIVE Advanced Combustion and Emission Control Roadmap</u>

- Incomplete understanding of the dynamics of fuel-air mixture preparation
- Incomplete understanding of stochastic combustion problems (CCV, misfire, knock)

<u>PACE Major Outcome 8</u>

- Understand and improve dilute combustion strategies during cold start and cold operation to reduce emissions

Partners

- **PACE is a DOE-funded consortium of 6 National Laboratories working towards a common goal (ACE138)**
  - Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, and more
- **Specific partners on this work include:**
  - LLNL on surrogate development and kinetics
  - Nek5000 development team at ANL, UIUC
  - PELE development team at LBNL, NREL, ORNL, SNL
  - Additional details on later slides

Relevance

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PACE Purposes in ACE138

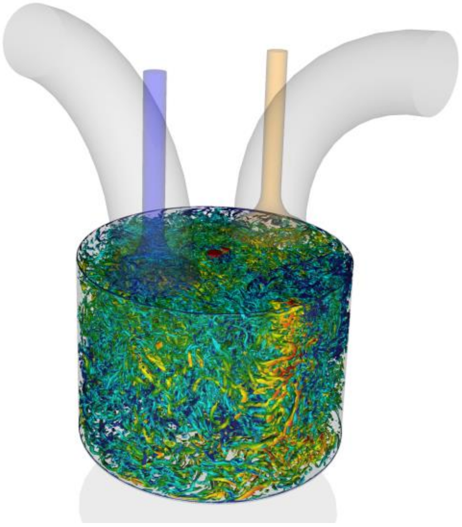
Overall Relevance of PACE:

PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions

Presentation Specific Relevance:

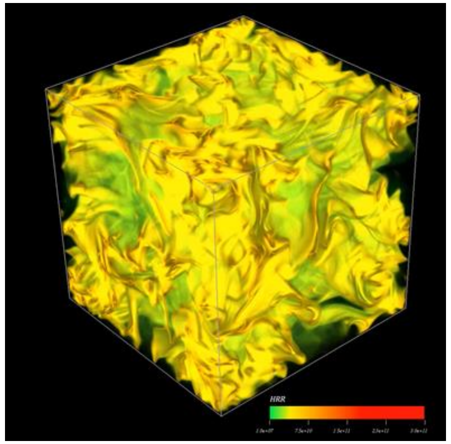
Unlocking high-efficiency dilute combustion by cyclic variability mitigation

- Modeling tools can be used to identify sources of CCV and develop and evaluate potential mitigations
- To accurately predict CCV, the CFD tool needs to accurately predict cycle-to-cycle variations in in-cylinder flow and mixing processes – needs high fidelity simulations



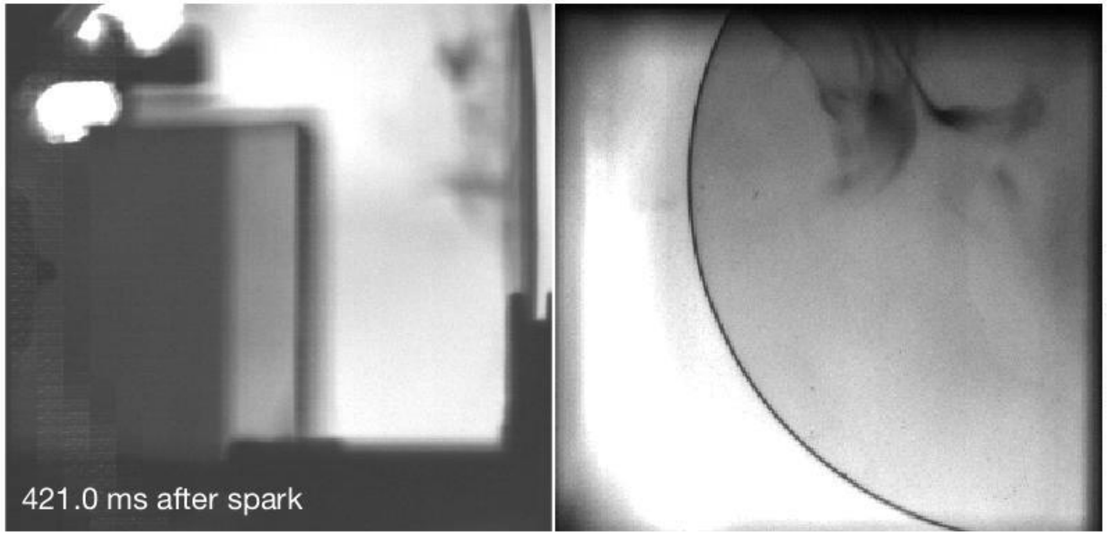
Better prediction of Cold Start Emissions

- Current submodels for combustion and emissions lack accuracy under cold-start operating conditions
- High-fidelity DNS using realistic fuel surrogates under cold-start conditions can complement experiments
- These datasets will be valuable for developing submodels for ignition, flame propagation, end-gas ignition, flame-wall interaction, and emissions



Relevance: Need for more predictive emission models

- **Major objective: develop predictive emission models using multi-fidelity simulation approach (LES/DNS) with extensive experimental validation**
- **Assessment of baseline simulations to identify key weaknesses in each standard sub-models used by industry – CONVERGE will be used**
  - Skeen and Yasutomi (2018) pyrolysis experiment to understand soot onset and inception
    - Accuracy of current model to predict thermal pyrolysis process and formation of soot precursor?
    - Is the current one-way coupling phenomenological soot model sufficient?
  - Soot film simulation of Sandia constant-volume chamber
    - Can the current approach predict successful spark ignition and subsequently premix propagation?
    - Spray wall impingement simulation ability to predict wall film formation
    - Is soot from wall film the product of pool fire combustion or fuel film pyrolysis?



Soot wall film experiment (Pickett & Skeen, SNL)

Video:
Left figure: side view of spray impingement from left to right
Right figure: behind the transparent wall
Physical process:
1.) Fuel spray impingement on the transparent wall (t=194.5 ms – 213.5 ms)
2.) Propagating premixed flame from top down (t=213.5 ms – 308. ms)
3.) First soot on-set at 308 ms

Milestones

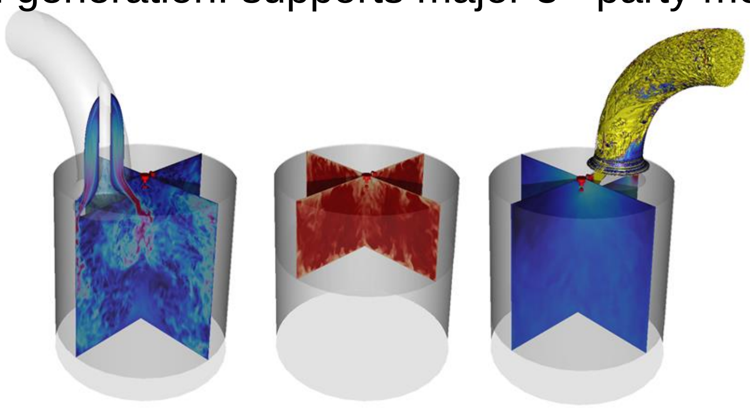
Month/Year	Description of Milestone	Status	Lab
Q4 FY19	Perform multi-cycle LES of motored TCC-III engine at 500 and 800 rpm	80% complete [delayed to Q3 FY20]	ANL
Q2 FY20	Complete implementing spray models and validate with benchmark experiments	On track	ANL
Q3 FY20	Complete implementing ignition, and flame propagation models and validate with benchmark flame experiments	On track	ANL
Q4 FY20	Perform multi-cycle LES of the Sandia optical DISI engine under motored operating condition	Delayed to Q2 FY21	ANL
Q1 FY20	Pyrolysis simulation	On Track	Sandia
Q2 FY 20	Sandia Chamber Pre-burn Simulation	On Track	Sandia
Q3 FY20	1D DNS of soot wall film	25 % complete	Sandia
Q3 FY20	1D DNS flame wall interaction (CONVERGE & S3D)	Setup validation	Sandia

Approach: DNS/LES Codes to Support Submodel Development

Nek5000

High-fidelity DNS/LES of ICE flows

- Spectral element method (**SEM**)-based spatial discretization delivering minimal numerical dispersion and dissipation and **exponential grid convergence**
- Semi-implicit and characteristic-based schemes (up to 3rd order accurate) for time-stepping
- Body-fitting capabilities for **complex geometries**
- Arbitrary Lagrangian Eulerian (ALE) capabilities to handle **moving boundaries**
- Capability to model fuel sprays and combustion
- Mesh generation: supports major 3rd party meshing tools

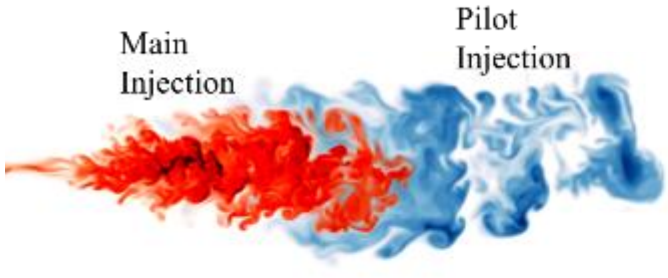


ECP Pele Combustion Codes

Exascale DNS and hybrid DNS/LES

- Time-dependent, adaptive mesh refinement (**AMR**) for large ranges of spatial and temporal scales in ***turbulent reacting flow***
- Engine-relevant **geometry**
- Agile, performant computational kernels
  - Thermo, transport, chemistry (+ data)
  - Soot production/dynamics models
  - Radiation interactions/transport
  - Spray/fluid coupling models
- PeleLM: AMR low Mach reacting flows
- PeleC: AMR compressible reacting flows

ECP
EXASCALE COMPUTING PROJECT



ECP investments in both codes make them scalable on upcoming exascale platforms

Approach: Leverage heavy ASCR investments in these codes to achieve **PACE objectives**

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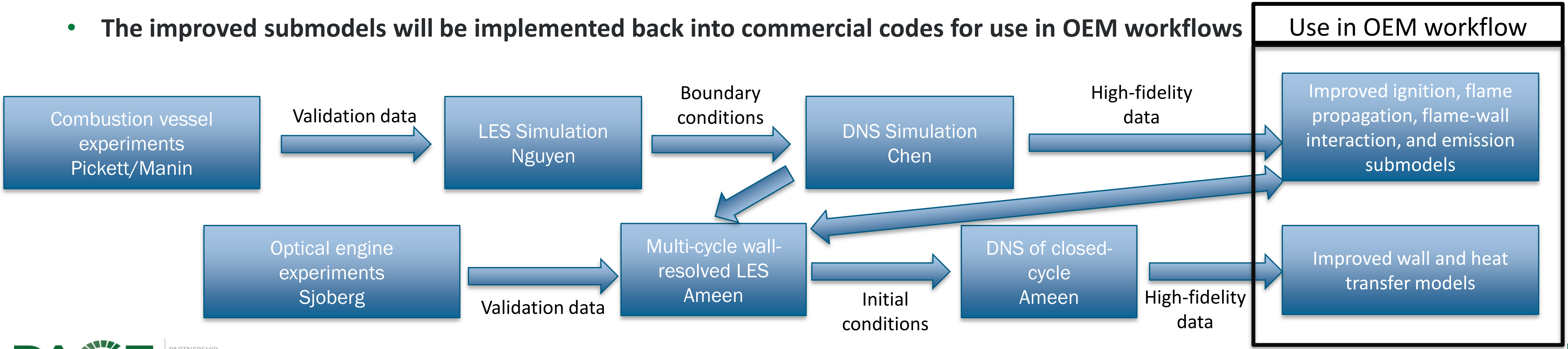
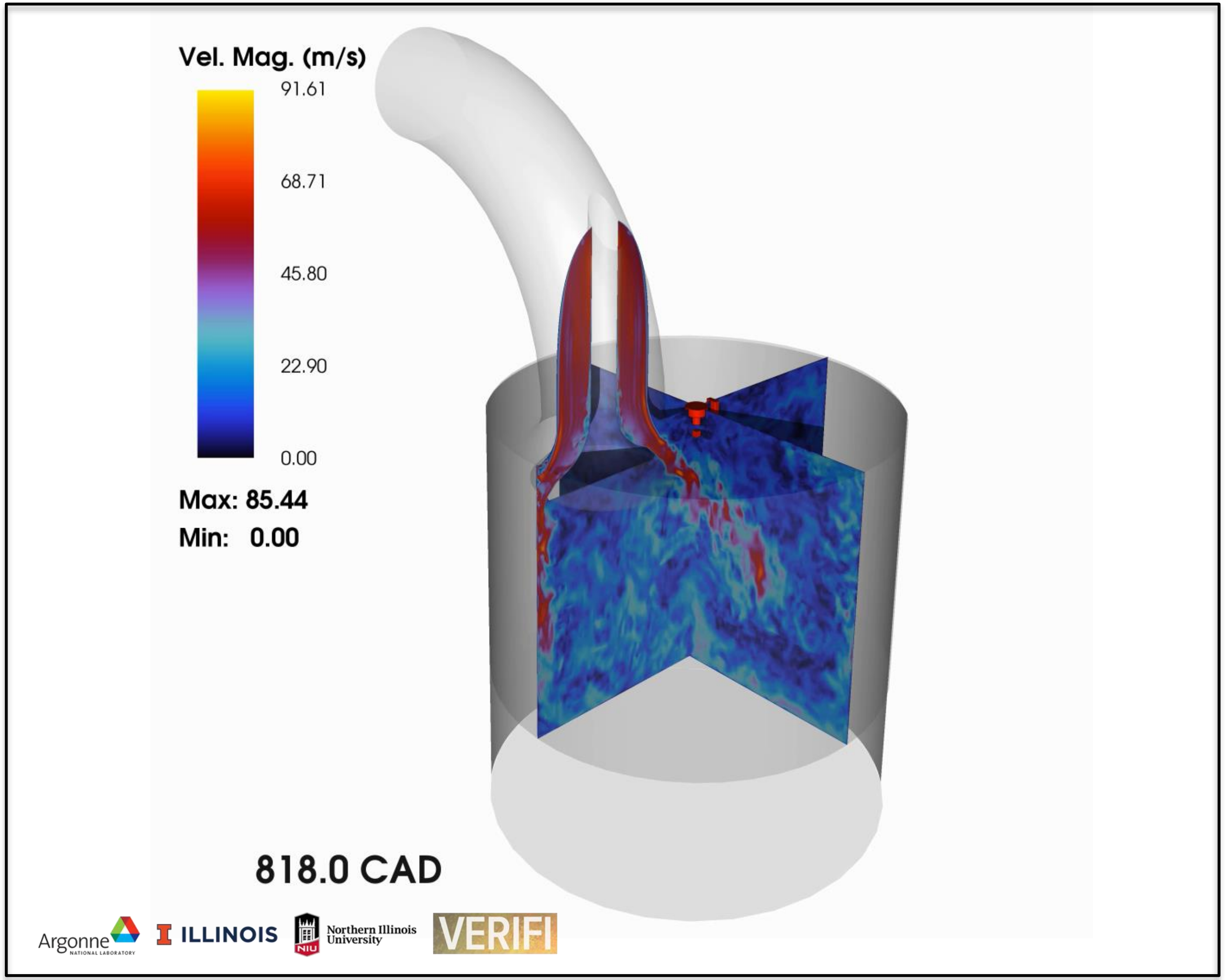
Approach

- **Adapt Nek5000 code into a simulation platform tailored for ICE simulations (ANL)**
  - Provide an accurate platform for testing and developing ICE-specific turbulence, spray and combustion submodels
  - Perform multi-cycle, high-fidelity wall-resolved LES to identify the root causes of cyclic variability and provide the understanding needed to design for their minimization
  - DNS of compression and expansion strokes to evaluate and improve wall and heat transfer models
- **Multi-fidelity approach for improved combustion and emission models (SNL)**
  - 1D and 2D DNS for large parametric variations to gain physical insight
  - Full 3D DNS simulations to provide high-fidelity and high quality data for developing submodels for ignition, flame propagation, flame-wall interaction, and emissions
  - Physics-based and data-driven sub-model development for both RANS/LES
- **The improved submodels will be implemented back into commercial codes for use in OEM workflows**



Accomplishment: Performed Multi-Cycle Wall-Resolved LES of TCC-III Engine (1/2) (ANL)



Visualization of the velocity, temperature, and λ_2 iso-surfaces during 1 full cycle of the TCC-III engine under motored conditions at 800 RPM

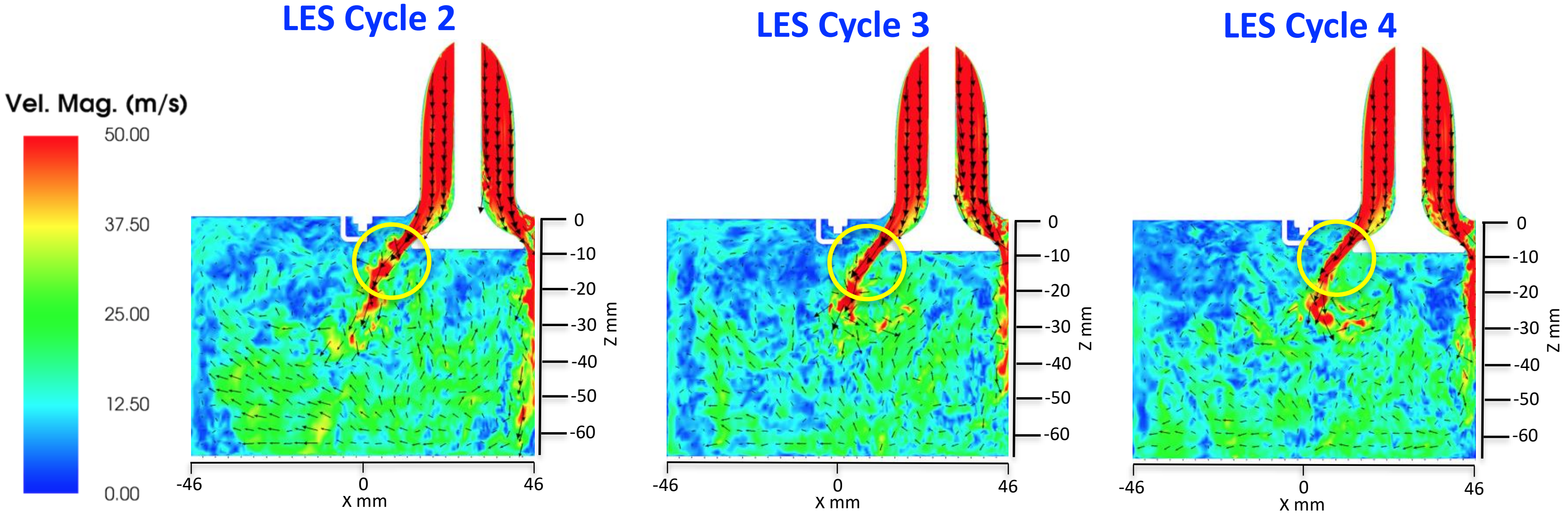
Wall-Time Per Cycle (720 CADs)	4.8 Days (with I/O)
Avg. Wall-time per CAD	9.7 minutes
Polynomial Order	5
Element Count	135K – 456K
Number of grid points	**29.2M - 98.5M**
Avg. Grid Sizes (Int/Exh)	~0.14mm
Avg. Grid Sizes (Comp/Exp)	**~0.08mm** @ 360 CAD aTDCexh **0.137mm** @ 230 CAD aTDCexh
Total CPUs	**16,384 cores**
HPC Platform	Theta (ALCF)

- Multi-cycle wall-resolved LES of the TCC-III engine under motored conditions at 800 RPM performed on ALCF Theta using ALCC allocation of 40M core hours
- Overset methodology with fixed mesh around spark plug and moving mesh elsewhere
- Well-resolved mesh in the valve opening and spark plug gap
- >80% scalability demonstrated on >16,000 processors for the engine simulation

Previous studies of the TCC-III engine from the PI:
Ameen MM et al. (2015) ASME ICEF
Ameen MM et al. (2016) IJER 18(4): 366-377

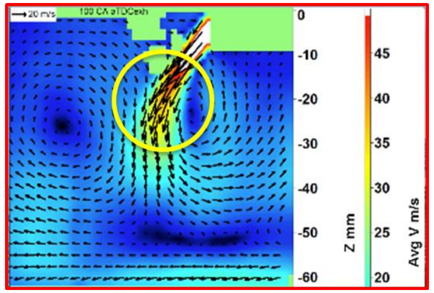
Accomplishment – Performed Multi-Cycle Wall-Resolved LES of TCC-III Engine (2/2) (ANL)

Velocity distributions @ **100 CAD aTDCexh** from Nek5000 and PIV measurements



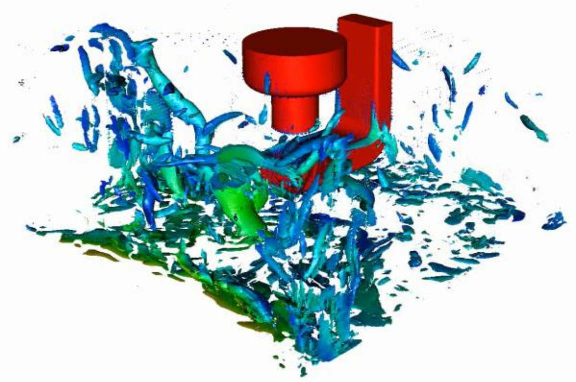
Mean PIV from UMich experiment

*Schiffmann, P., Sick, V., Reuss, D. (2018) https://doi.org/10.7302/Z2MS3QP3



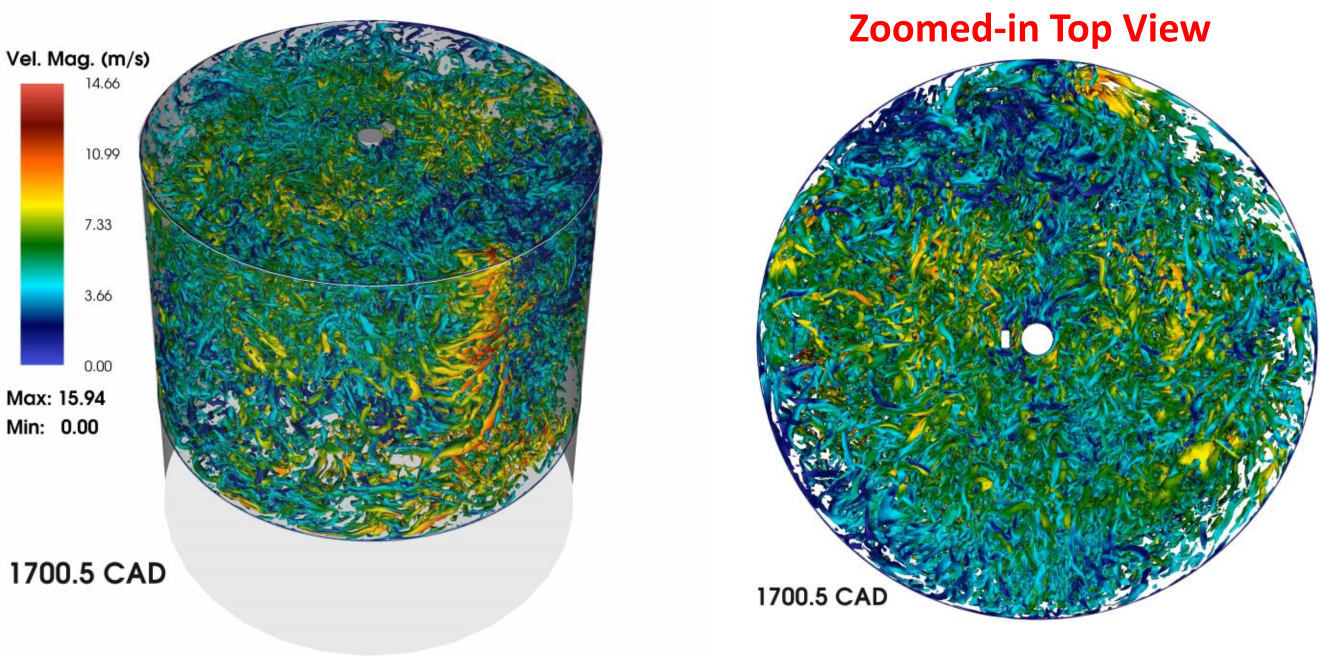
Preliminary results show qualitative similarity in jet penetration and orientation

- Simulations still in progress (10 cycles planned; 5 completed)
- Simulation validation using PIV measurements from UMich
- Multi-cycle dataset will be used to evaluate causes of CCV and develop better wall models for LES
- Next Step:
  Apply the same procedure for Sandia optical DISI engine under motored and fired conditions



- Flow features showing interaction of the intake jet with the spark plug
- Vortex shedding from this interaction could be a factor affecting CCV – Needs validation using experimental data

Accomplishment – Performed First Ever DNS of Motored Engine Flows (ANL)



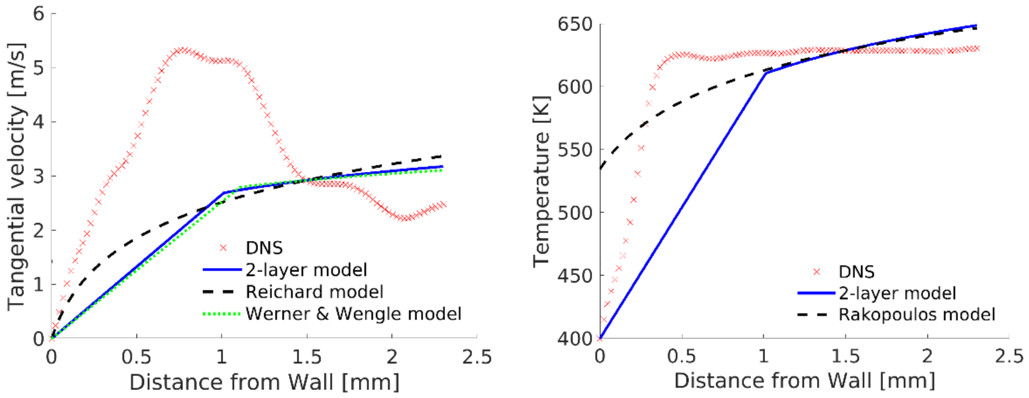
Visualization of the λ_2 iso-surfaces during the compression stroke showing the appearance of smaller scale flow features as the piston moves up

- Demonstrated the capability to perform DNS-level simulations for the TCC-III compression stroke on more than 50k processors
- Conventional wall models shown to be inaccurate to model wall shear stress and heat flux
- Next Step: Improve accuracy of wall models in engine simulations (in collaboration with P Pal (ANL) and M Ihme (Stanford))

Largest ever engine simulation

Wall-Time for100 CADs	1.91 Days (with I/O)
Avg. Wall-time per CAD	27 minutes
Polynomial Order	9
Element Count	321K to 416K
Number of grid points	321M to 416M
Avg. Grid Sizes (Comp/Exp)	~0.02mm @ 360 CAD aTDCexh 0.037mm @ 230 CAD aTDCexh
Total CPUs	**51,328 cores**
HPC Platform	Theta (ALCF)

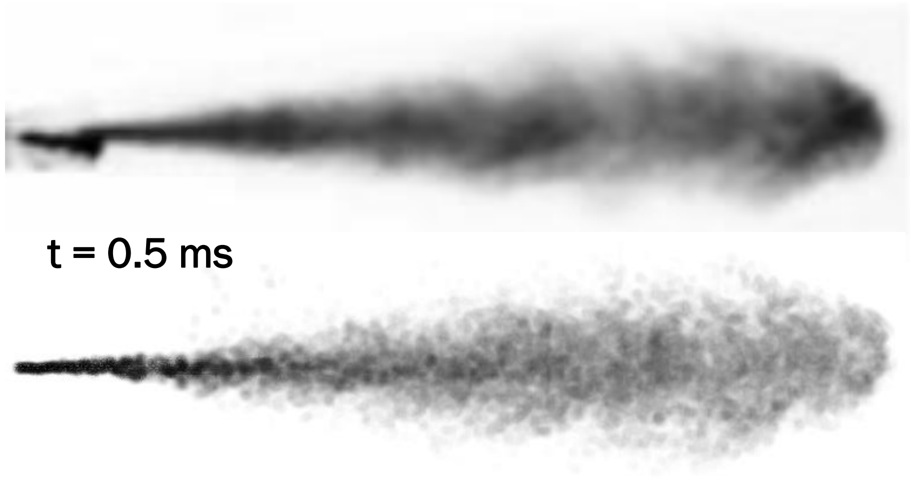
Evaluation of the accuracy of wall models using DNS dataset



- The DNS dataset was extracted at points normal to the cylinder head at x=0, y=28mm at CAD320
- Wall model profiles obtained by matching velocity and temperature with DNS at 1.5 mm

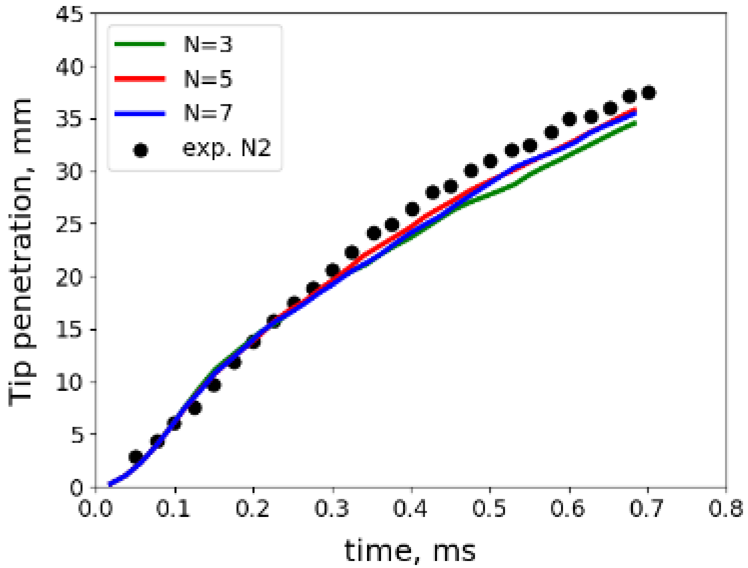
Accomplishment – Performed LES of Non-Evaporative Spray (1/2) (ANL)

- Spray models implemented into Nek5000 by leveraging significant expertise (modeling and X-ray diagnostics) within the ANL Spray team
- A Parallel Particle In Cell Library in Fortran (ppiclF*) has been coupled with Nek5000 to model two phase flows in an Eulerian Lagrangian framework.
- LES of non-evaporative sprays were conducted in the low-Mach framework using Nek5000.
  - Experimental conditions in Margot et al. (2008) were simulated.
- Numerical results for liquid penetration show excellent agreement with experimental data.
- Grid-convergent results were achieved by increasing N, which are difficult to obtain in low-order codes.
- Qualitative comparison with experimental images shows good agreement in spray shape and angle.



Top: shadowgraphy of experimental spray.

Bottom: Volume rendering of projected particle volume fraction.



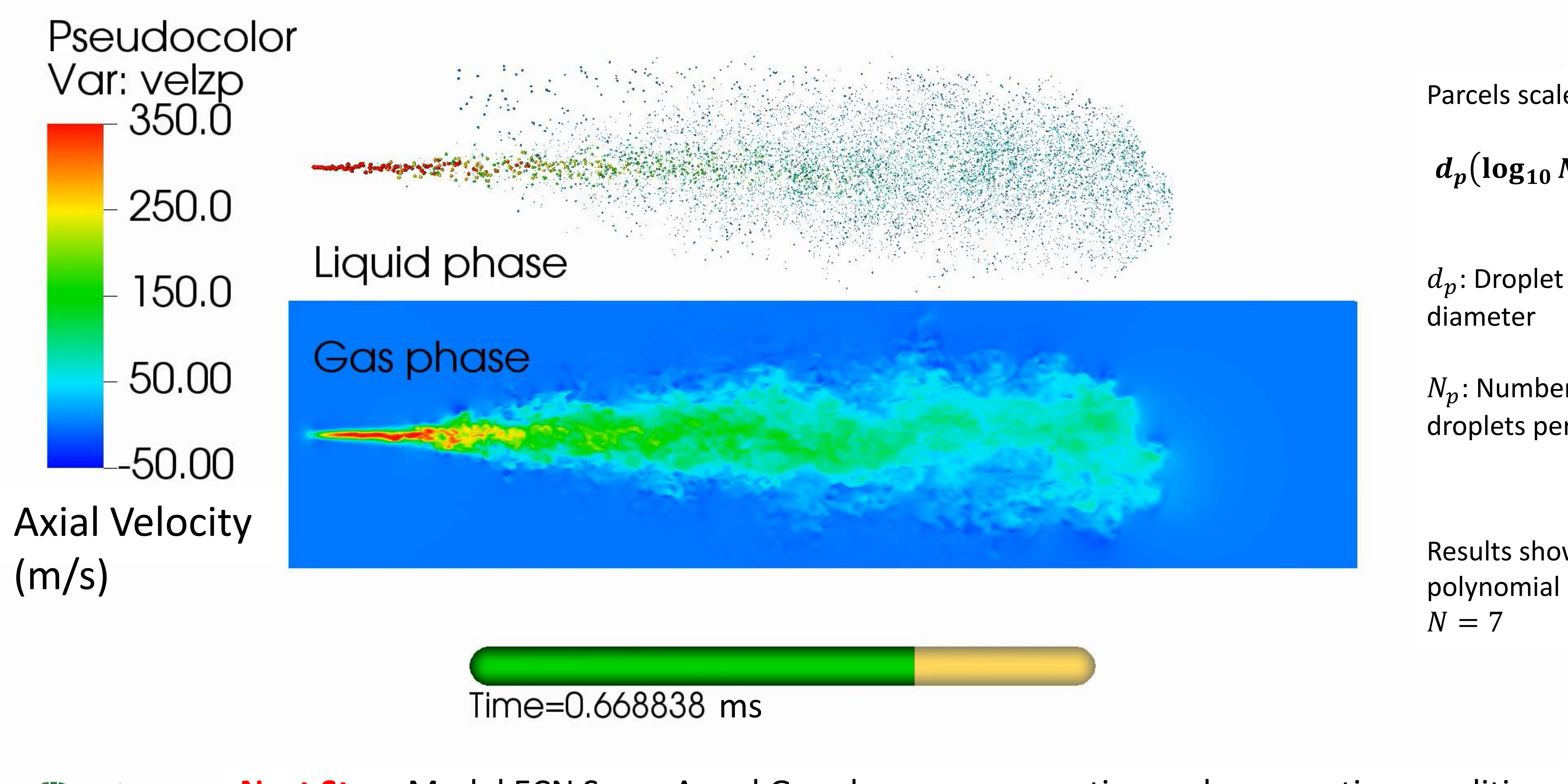
Grid convergence of liquid (tip) penetration

Nozzle Diameter	140 μm
Injection pressure	80 MPa
Ambient pressure	2 MPa
Ambient gas	Nitrogen
Fuel	Diesel

# elements	22,570
Max # parcels	~ 52,000
Wall time ($N = 5$):	5 h
# CPUs	576

* https://dpzwick.github.io/ppiclF-doc/algorithms/performance.html

Accomplishment – Performed LES of Non-Evaporative Spray (2/2) (ANL)



Axial Velocity (m/s)

Parcels scale:

$$\boldsymbol{d_p}(\mathbf{log_{10}}\,\boldsymbol{N_p} + \mathbf{1})$$

d_p: Droplet diameter

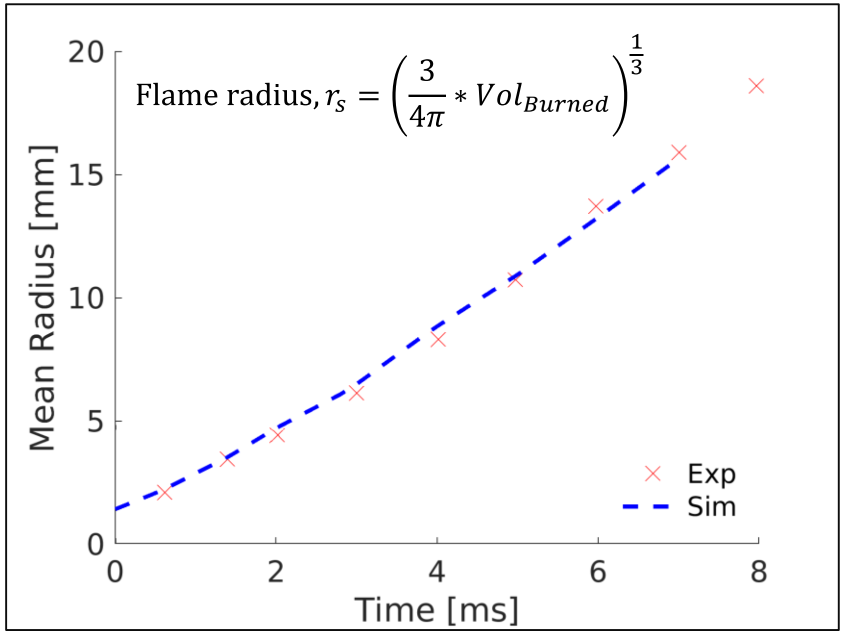
N_p: Number of droplets per parcel

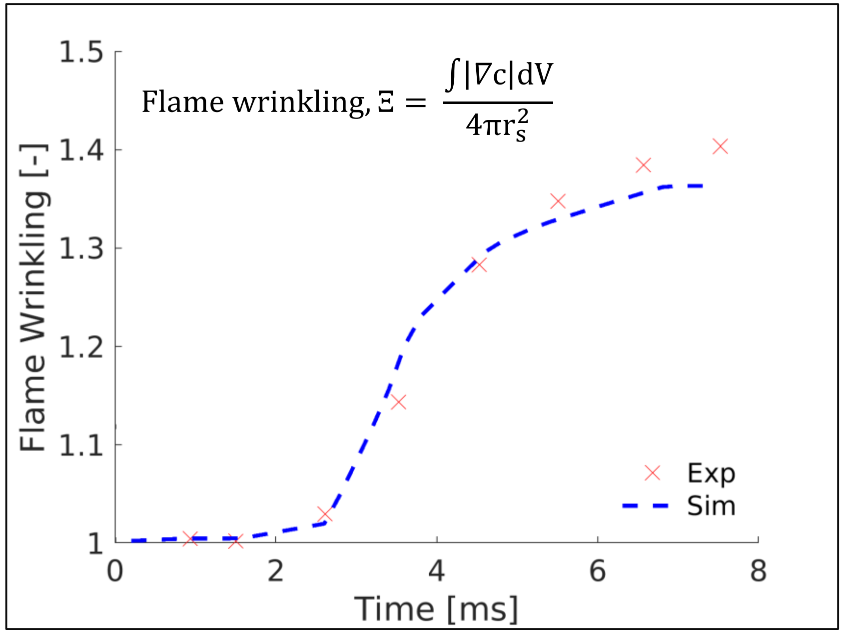
Results shown for polynomial order $N = 7$

Next Step: Model ECN Spray A and G under non-evaporating and evaporating conditions

Technical Accomplishment – Combustion Modeling with ECFM (ANL)

- The extended coherent flamelet model (ECFM) was implemented as a turbulent premixed combustion model in Nek5000
- Implementation validated for a turbulent premixed flame propagation for a propane-air mixture
- A stoichiometric propane-air flame propagates in a turbulent field characterized by u_0/S_l = 0.9 and l_t = 6.5 mm.
- Flame is initialized using a sphere of radius 1.5 mm





Validation for spherical turbulent premixed propane-air flame against experimental data from Renou and Boukhalfa (CST, 2001).

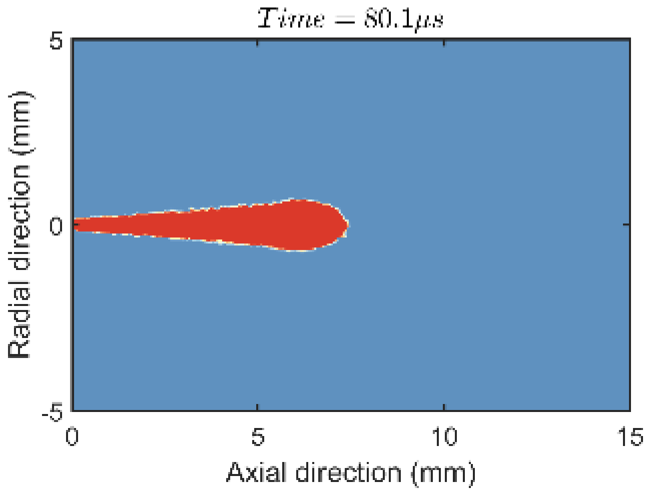
Overall, ECFM model is able to capture the flame propagation under isotropic turbulence reasonably well

Next Steps:

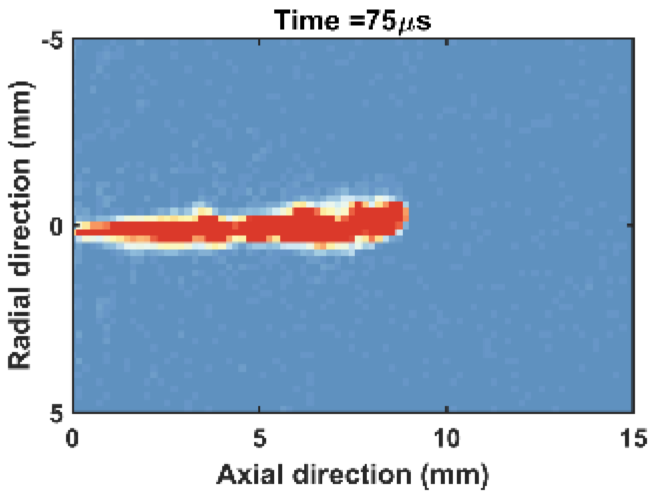
- Further validation using 2D and 3D DNS results from Sandia's 2014 study on HCCI/SACI combustion – more challenging condition
- Dataset from upcoming DNS task from Sandia (PI: Chen) will be used to improve the flame propagation and flame-wall quenching submodels in ECFM under engine-relevant conditions
- ECFM with improved submodels will be ported into commercial codes as part of the PACE coordination tasks

Accomplishment: Current soot model cannot capture soot onset and behavior (SNL)

- **Modeling pyrolysis experiment of Skeen and Yasutomi (2018)**
  - Ambient condition: P=76 bar, T=1500 K, 0% oxygen
  - Soot formation mainly due to pyrolysis, no soot oxidation
  - 100 µs injection duration, minimized soot turbulence interaction
  - 2 different mechanism: Wang & Reitz (100-species) and Narayanaswamy (255 species)
  - To understand the current model capability, no constant tuning was performed
  - One-way coupling phenomenological soot model with Pyrene (A4) as the soot precursor
    - One way coupling: soot formation will not affect gaseous chemistry (no gas-to-soot species conservation is enforced)
  - Effect of one-way coupling
    - Exponential soot growth due to the lack of species conservation once soot is formed
    - Dominate surface growth mechanism because of C2H2
- **Next step: provide vaporized initial conditions for DNS study using PeleC and recently developed Hybrid Method of Moments**

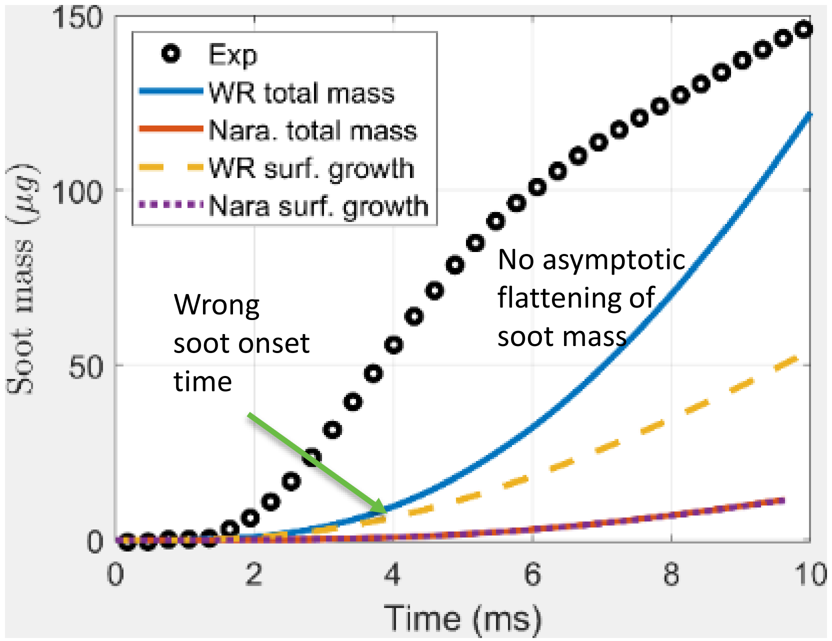


Projected Liquid Volume



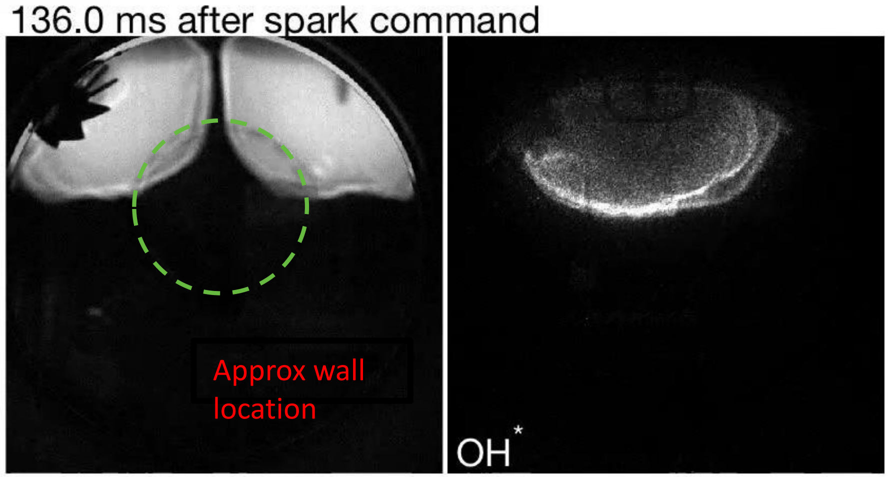
DBI spray image (Pickett & Skeen)

Qualitative image shows good agreement between simulation and experimental spray penetration

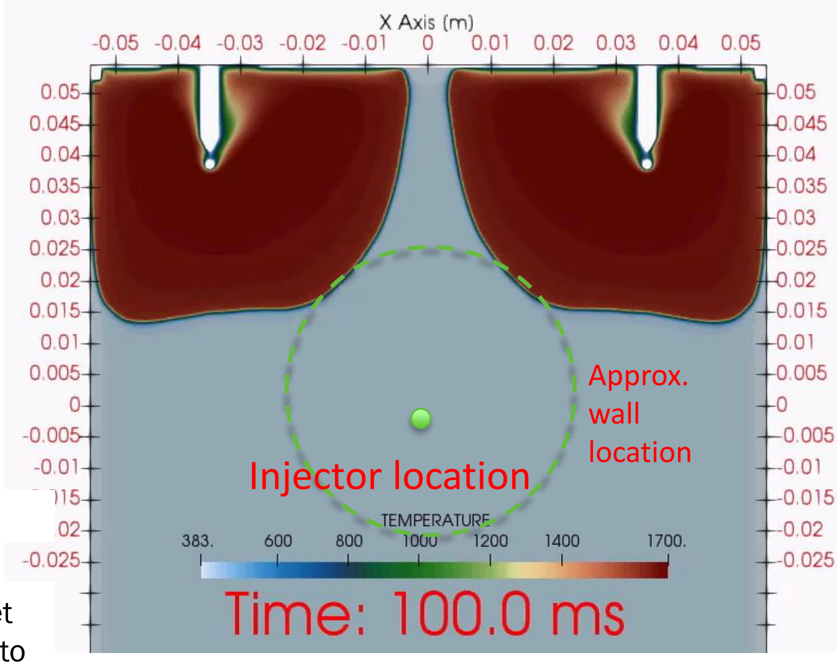


Accomplishment: Understanding chamber pre-burn for soot wall film experiment (SNL)

Quiescent initial condition with 3.2 % C_2H_2, 0.5% H, 8.25 % O_2, 88.05 % N_2 by volume.
CONVERGE SAGE solver (finite rate chemistry):
73 species C2H2 mechanism
Captures differential diffusion effect
3 consecutive sparks with 80 mJ total energy, 12.5 ms total duration

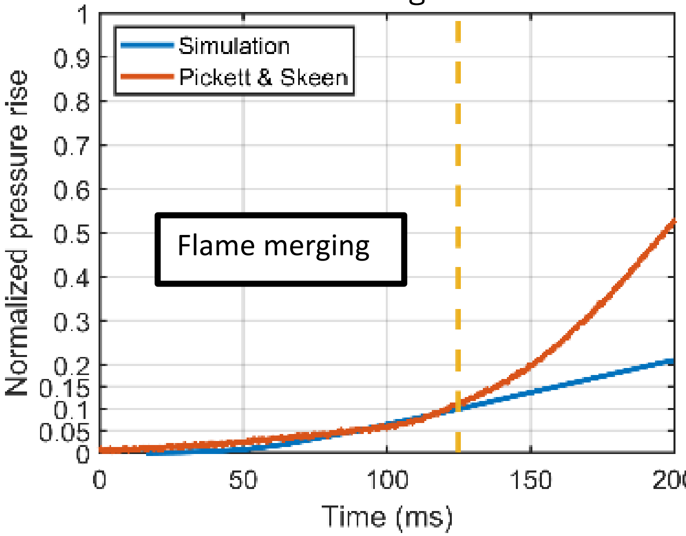


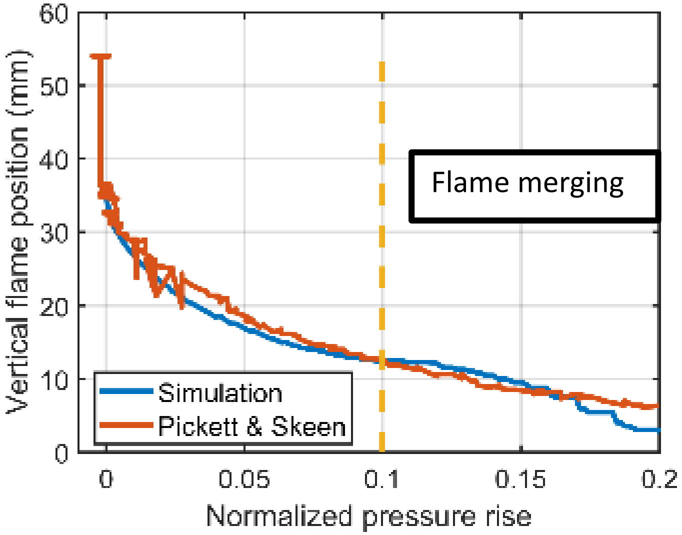
Same experiment from different view (Pickett & Skeen, SNL)



- Simulation does not include a wall
- Pre-burn simulation to first understand flame propagation characteristic
- During flame merging, flame position stagnates, evidence by both simulation and experimental observation
- Simulation can capture the flame position as a function of the normalized pressure rise, yet fails to predict the true pressure rise within the chamber, especially after flame merging occurs.
- How to account for mixing fan effect?
- Flame propagation is sensitive to thermal and composition stratification (Bhagatwala et al. 2014 (SNL))

Experimental pressure curve is offset to the first instance of pressure rise to match simulation timing



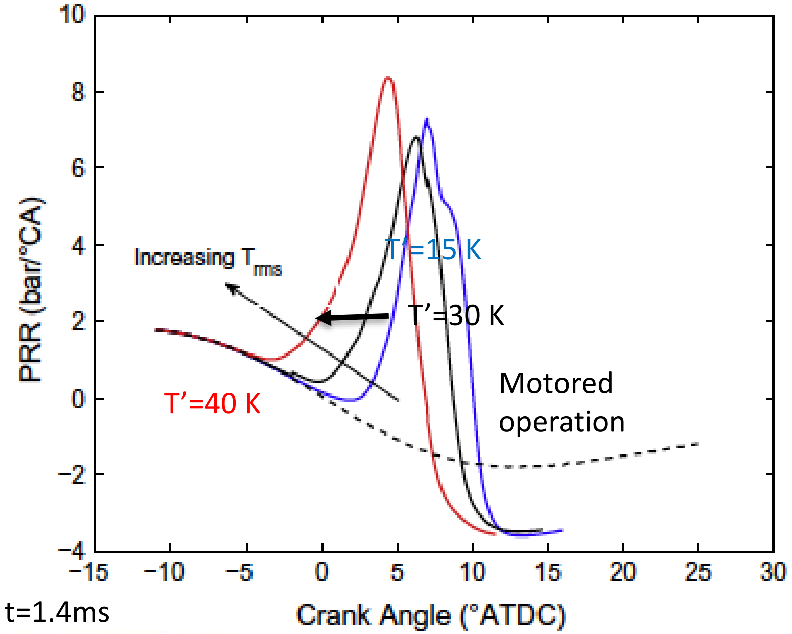


Background: established flame propagation speed dependency on thermal and composition stratification under SACI conditions from early DNS

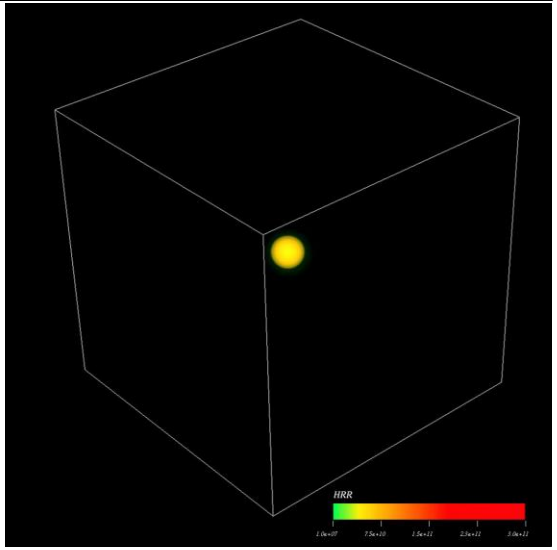
Used 2D/3D DNS to study stratification effects on propagation speed in ethanol SACI DNS with S3D on Titan at OLCF

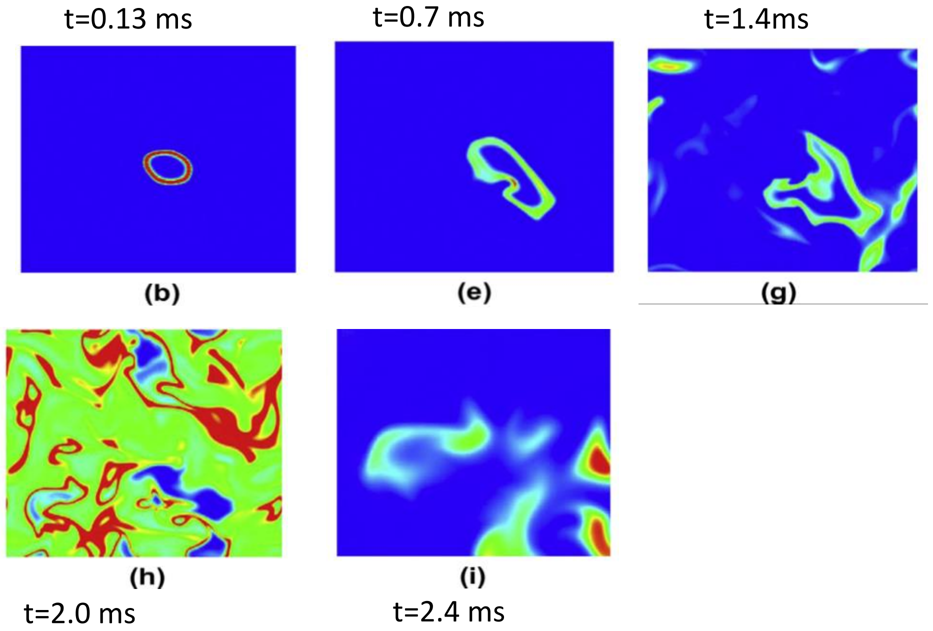
(***Bhagatwala et al. 2014)***

Ethanol propagation speed strongly depends on thermal and composition stratification, higher stratification results in faster pressure rise rate, which modulates combustion phasing



3D DNS with S3D, heat release





Heat release rate isocontours in one slice through the DNS data show early flame attenuation and eventual extinction before end gas autoignition

Adaptive Mesh Refinement in Pele will enable much larger domains and higher Reynolds no. for DNS of SACI with surrogate gasoline fuel

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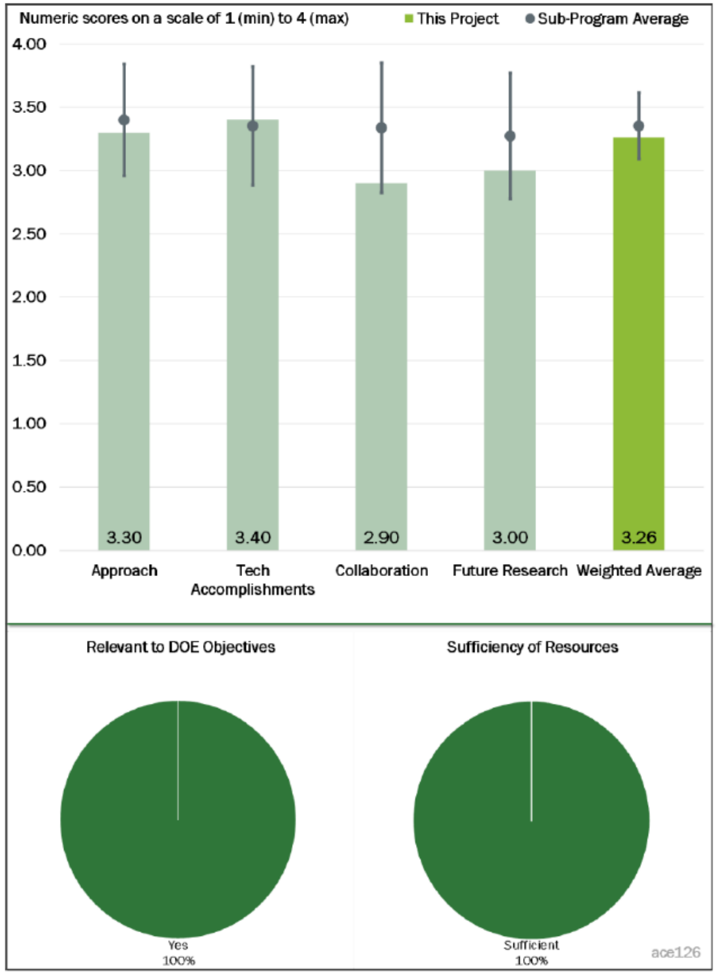
Response to Previous Year Reviewer's Comments

ACE146 (Ameen, ANL) was the only project funded and reviewed in FY19



- It was unclear to the reviewer how developments from this program will be passed onto commercial code vendors for incorporation into the fully supported, production-engine simulation software needed by engine developers.

Under the PACE program, the improved submodels generated as part of this project will be ported into commercial CFD codes which the industry can use. Also, the detailed dataset generated from these simulations which provides valuable info about the in-cylinder flow structures will be available to the industry.

- The reviewer indicated that collaboration with a company like Pointwise for mesh generation may be valuable for this effort.

Collaborations with Pointwise Inc. have been started in FY20 for better and faster meshing techniques.

- The reviewer asked if there is any plan to look at wall-boundary layers to improve law-of-the-wall formulations

Wall-resolved LES results are now available and will be used to improve wall models. DOE FOA project with Stanford, UConn will investigate further into this.

Partnerships/Collaborations

PACE Collaboration

- Bill Pitz, Scott Wagnon (LLNL) – Skeletal/reduced mechanisms for PACE surrogates
- Russell Whitesides (LLNL) – Implement fast chemistry and transport solvers
- Lyle Pickett, Julien Manin (SNL) – Spray vessel experiments
- Magnus Sjoberg (SNL) – Optical engine experiments

External Collaborators

- Pointwise Inc. – Fast and efficient mesh generation for Nek5000
- Paul Fischer (UIUC) – Solver development for compressible version of Nek5000
- Joe Insley, Silvio Rizzi (ANL-LCF) – Integrate in-situ visualization capabilities into Nek5000
- Kris Rowe (ANL-LCF) – GPU version of Nek5000
- Matthias Ihme (Stanford) – Implement non-equilibrium wall models in Nek5000
- Chao Xu, Pinaki Pal (ANL) – Submodel implementation in Nek5000
- PELE Team (LBNL, NREL, ORNL, SNL) – Submodel implementation and scalability in PELE

Remaining Challenges and Barriers

- **PACE-wide barriers discussed in ACE138**
- **Coupling with commercial CFD codes:**
  - Need to develop workflows to perform hybrid DNS/LES or LES/RANS simulations by coupling with commercial or open-source low-order CFD codes
  - Use data generated from DNS and wall-resolved LES simulations to improve submodels in commercial codes
- **Size and accuracy of skeletal/reduced mechanisms for PACE fuel surrogates:**
  - Collaborations with the PACE combustion/kinetics team to develop compact mechanisms (~100 species) with sufficient accuracy for the high-fidelity DNS simulations
- **Computational resources may be limited:**
  - ALCC and INCITE proposals to be submitted for access to DOE leadership class machines
  - Long queue times on leadership-class machines
- **Proper archiving of data:**
  - High fidelity simulations will generate >100 TB of data. There is a need to develop efficient data analytics and ML tools, and workflow to share this data across the PACE program

Proposed Future Work - ANL

Remaining Milestones for FY20

- Q2 FY20: Complete implementing spray models and validate with benchmark experiments [on track]
- Q3 FY20: Complete implementing ignition, and flame propagation models and validate with benchmark flame experiments [on track]
- Q4 FY20: Perform multi-cycle LES of the Sandia optical DISI engine under motored operating condition [delayed to Q2 FY21]

Proposed Future Tasks:

- Complete implementing spray, ignition, and flame propagation models and validate with benchmark experiments [FY20]
- Multi-cycle LES of the Sandia optical DISI engine [FY20-FY21]:
  - Improve understanding on causes of cyclic variability in flow, mixing, spray and combustion
  - Archive numerical setup, flow and thermal data
- Improve submodels for flame propagation and flame-wall quenching using Chen’s DNS dataset
- Develop an open-source platform that industry/academia/national lab PIs can use for submodel development

Any proposed future work is subject to change based on funding levels

Proposed Future Work - SNL

- **CONVERGE Constant-volume chamber simulation (Nguyen, SNL)**
  - Continue chamber pre-burn simulation for various ambient compositions, including a wall based on experimental design of Pickett, SNL
  - Spray wall impingement simulation and side wall flame quenching of the new configuration
  - LES of flame wall interaction (1D- 3D) of both wet/dry wall and provide boundary conditions for DNS studies (Chen, SNL)
- **S3D 1D-2D DNS of flame-wall interaction for a range of fuels: hydrogen, methane/hydrogen, iso-octane, and gasoline surrogate (Chen, SNL)**
  - Wet/dry wall effects, including fuel dilution, equivalence ratio and fuel stratification variation
  - Pyrolysis and soot reactions from wall film
  - End gas auto-ignition (knock)
- **PeleC 3D DNS of SACI with iso-octane and gasoline surrogate (Chen, SNL)**
  - Early kernel growth, flame propagation, and end-gas ignition

Any proposed future work is subject to change based on funding levels

Summary

Relevance

- Cyclic variability mitigation and reducing cold start emissions are barriers to attaining higher efficiency for dilute SI combustion

Approach

- Leverage ASCR funded codes Nek5000 and Pele to perform high-fidelity simulations of the flow, spray and combustion processes in SI engines
- Adapt Nek5000 code into a simulation platform tailored for ICE simulations
- Multi-fidelity approach for improved wall heat transfer, combustion and emission models

Accomplishments

- Performed multi-cycle LES of the motored TCC-III engine and
- DNS of the compression/expansion stroke performed on >400M grid points on >51,000 processors - Largest ever engine simulation
- Implemented spray submodels in Nek5000 and demonstrated the accuracy in modeling non-evaporating sprays
- Implemented ECFM combustion model in Nek5000 and modeled turbulent premixed flames
- Demonstrated that one-way coupled soot models cannot capture soot onset or growth under pyrolysis conditions
- Simulated the chamber pre-burn for soot wall film experiment

Future Work

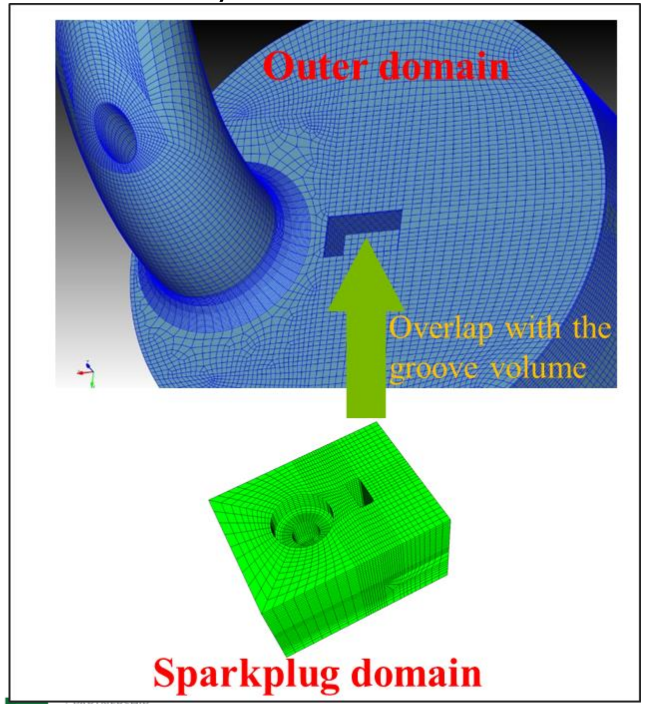
- Multi-cycle LES of the Sandia optical DISI engine
- Improve combustion submodels in Nek5000 using Chen's DNS dataset
- S3D 1D-2D DNS of flame wall interaction for a range of fuel: hydrogen, methane/hydrogen, iso-octane, and gasoline surrogate
- PeleC 3D DNS freely propagating flame with iso-octane and gasoline surrogate

TECHNICAL BACKUP SLIDES

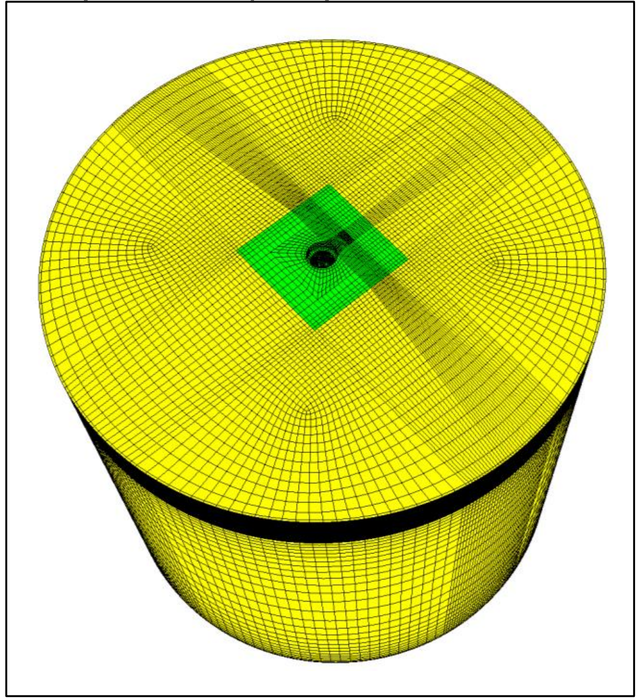
Engine Simulation Workflow on Nek5000

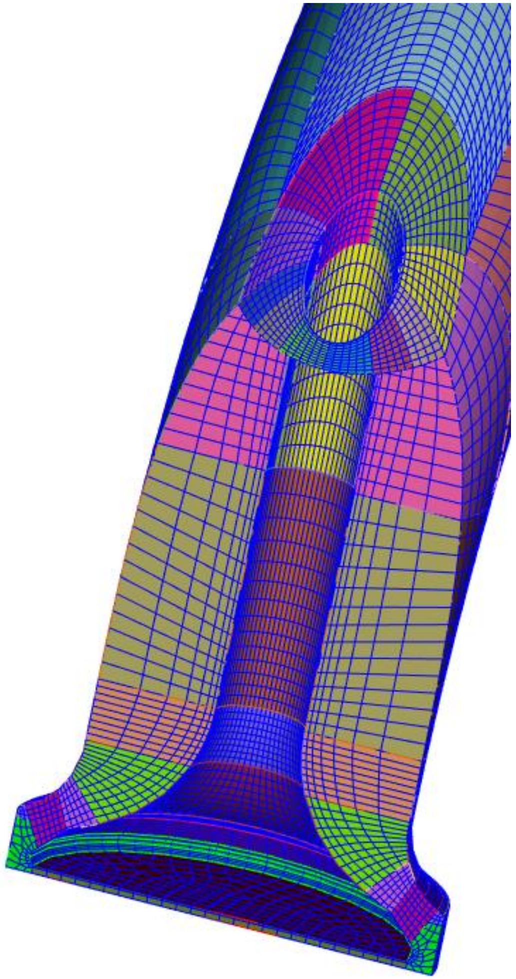
Intake Stroke	Compression/Expansion Stroke	Exhaust Stroke
• NekNek Overset mesh approach • Fixed mesh around spark plug and moving mesh outside spark • Minimizes mesh distortion	• Single Mesh calculation • Mesh motion prescribed using an affine transformation in the region between spark plug and piston	• NekNek Overset mesh approach • Fixed mesh around spark plug and moving mesh outside spark • Minimizes mesh distortion

Meshing Strategy for Intake/Exhaust Strokes



Meshing Strategy for Compression/Expansion Strokes





Mesh in the Intake Port

The ECP Pele Combustion Codes

(https://github.com/AMReX-Combustion)

Exascale DNS and hybrid DNS/LES

- Time-dependent, adaptive mesh refinement (**AMR**) for large ranges of spatial and temporal scales in ***turbulent reacting flow***
- Engine-relevant **geometry**
- Agile, performant computational kernels
  - Thermo, transport, chemistry (+ data)
  - Soot production/dynamics models
  - Radiation interactions/transport
  - Spray/fluid coupling models

PeleLM

AMR low Mach reacting flows
- Eliminates acoustics, large timesteps
- Required linear solvers, implicit chemistry

PeleC

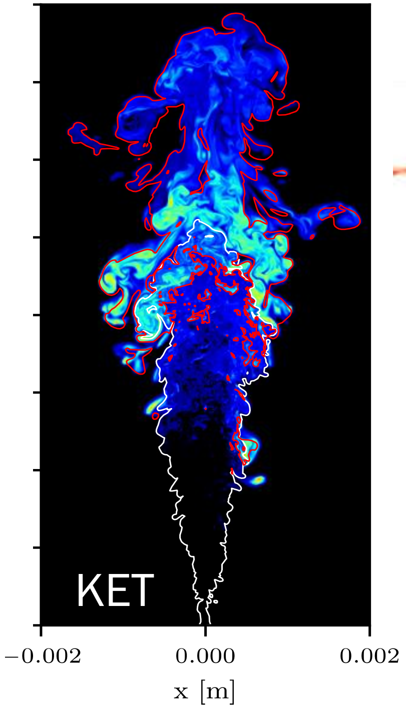
AMR Compressible reacting flows
- Time-explicit gas dynamics

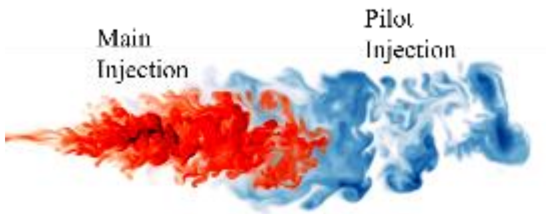
PelePhysics

Combustion models (chemistry, thermo, transport, spray, soot, radiation, etc)

Additional Pele modules

PeleC-MP	Particle integration/management
PeleAnalysis	Post processing, model-specific analysis, CEMA/reaction path analysis, in-situ tools, problem setup
PelePlot	AMR- and combustion-specific visualization tools
PeleRegressionTesting	Distributed, automated CI and regression management
PeleProduction	Collaboration hub

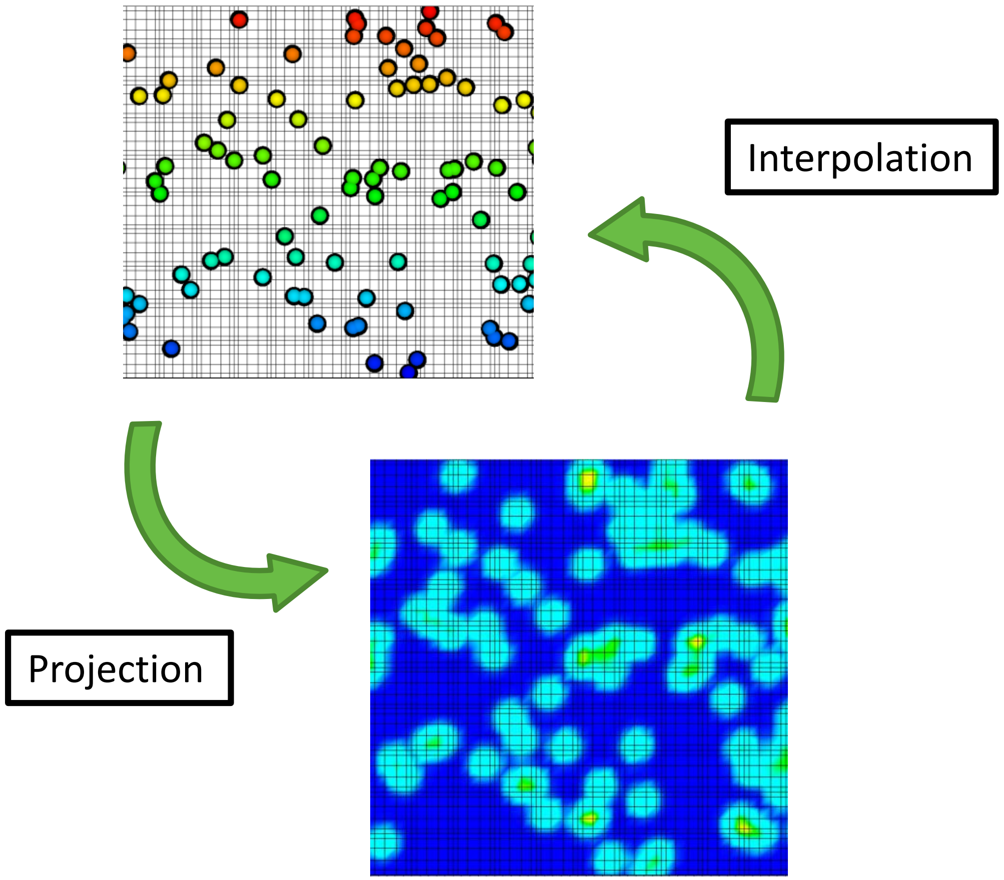




Eulerian/Lagrangian method for Modeling Fuel Sprays

- **Carrier phase**
  - Eulerian field, solved using Nek5000.
  - Low-Mach formulation
- **Suspended phase**
  - Lagrangian field, solved using PPICLF.
  - Strong Stability Preserving (SSP) RK3 used for explicit time-stepping.
  - Groups of droplets are represented by parcels.
  - Blob injection method used to model liquid injection.
- **Two-way coupling**
  - Spectral interpolation of gas properties at parcel locations for the computation of momentum, heat and mass transfer.
  - Momentum, heat and mass source term projection onto Nek5000 grid using Gaussian filter of finite width.
- **Droplet breakup**
  - Kelvin-Helmholtz model for primary breakup.
  - Rayleigh-Taylor model for secondary breakup.
- **Droplet dynamic drag**
  - TAB model used to account for droplet distortion.

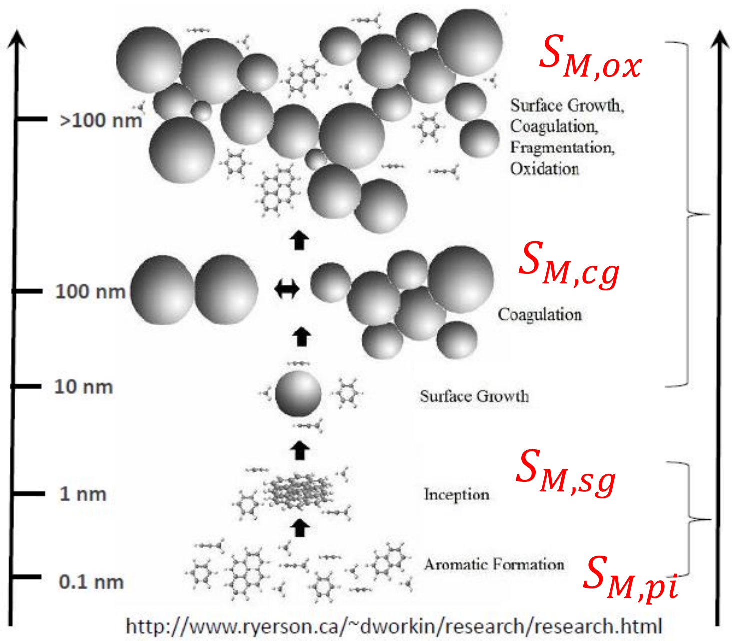
Parcels colored by interpolated gas velocity in a Couette flow



Eulerian field colored by projected particle volume fraction

Soot Modeling Overview

- **One-way coupling soot model (popular in industry)**
  - Empirical
    - Calculate averaged soot mass
    - Only include inception (Hiroyasu)and oxidation (NSC)
  - Phenomenological soot model
    - Soot mass and number density
    - Include all major process
  - Precursor species to soot conservation is not enforced
- **Two-way coupling soot model**
  - All major physiochemical processes are enforced
  - Method of Moments: soot mass, number density, volume fraction
  - Sectional Method: particle size distribution function, soot mass, number density, volume fraction



Source: CONVERGE 2.4 manual

Higher fidelity

Increase computational cost

- Sectional Method (Particulate Size Mimic)
- Method of Moments (Particulate Mimic) **
- Phenomenological *
- Empirical

*: Project starting point
**: Project end goal

General soot governing equation

$$\frac{DM}{Dt} = S_M$$

$$S_M = S_{M,pi} + S_{M,sg} + S_{M,cg} + S_{M,ox}$$

M: soot mass, number density, moments
S: soot physiochemical source term

ECFM Combustion Model

- The extended coherent flamelet model (ECFM) was implemented as a turbulent premixed combustion model in Nek5000
- This involves solving transport equations for progress variable, $\tilde{c}$, and flame surface density, $\overline{\Sigma_c}$

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{u}\tilde{c}) = \nabla \cdot \left(\sigma_c \frac{\bar{\rho}\widetilde{\upsilon_t}}{Sc_t} \nabla \tilde{c} \right) + \rho_u S_l \overline{\Sigma_c}$$

$$\frac{\partial \overline{\Sigma_c}}{\partial t} + T_{res} + T_{sgs} = S_{res} + S_{sgs} + C_{res} + C_{sgs} + P$$

  - Here, T_{res}, S_{res}, C_{res}, P refers to transport, strain, curvature, and propagation terms due to resolved flow motions
  - T_{sgs}, S_{sgs}, C_{sgs} are the unresolved transport, strain, and curvature terms
  - $\tilde{c}$=1 refers to fully burned mixture and $\tilde{c}$=1 refers to unburned mixture

- The source term for fuel mass fraction, $\dot{\omega_F} = \overline{\rho_F}^u S_l \overline{\Sigma_c}$
- Thermodynamic properties estimated using Chemkin – assuming equilibrium in the burned mixture
- Current implementation is CFM. ECFM involves solving transport equations for a few major species to account for partially premixed mixtures and EGR